

Chapter 17 Quantification of Exposure: Chemical and Physical Properties Affecting Multimedia Fate and Transport

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17.1 Introduction

This chapter provides both an overview of the physical and chemical properties of chemicals that persist in the environment long enough to be of potential concern for multimedia exposure and information on their potential to bioaccumulate in biological tissues to levels that may result in significant exposures. This chapter also provides a brief discussion of various approaches for evaluating persistence and bioaccumulation in an air toxics exposure assessment.

- The term **persistence** refers to air toxics that are slow to degrade in the atmosphere or in the soils, water, and/or sediments onto which they deposit and partition. Under certain circumstances, persistent chemicals can increase in concentration over time. In addition, some of these pollutants can bind tightly to soils and sediment and move from place to place by erosion. Examples of persistent chemicals are metals (which never degrade) and polychlorinated biphenyls (which degrade, but only over very long periods of time). Measures of persistence are described in Section 17.1.1.
- The term **bioaccumulation** refers to persistent chemicals that build up in the tissues of living organisms to concentrations that are higher than in the surrounding environment. These pollutants are often lipophilic in nature, which allows them to be taken up in and stored by fat tissues. As an example, the group of chemicals known collectively as dioxins (usually some mixture of chlorinated dioxins and furans) persists for long periods of time in the environment and is strongly lipophilic. Repeated exposure to dioxin in food can lead to increased body burdens in fat tissue and human milk. Measures of bioaccumulation are discussed in 17.1.2.
- The term **biomagnification** refers to persistent chemicals that increase in concentration as they transfer up the food chain so that they accumulate to higher concentration levels with each successive food chain level (see Section 17.1.2).

The air pollutant's physical and chemical properties and the characteristics of the environment to which the pollutant is emitted affect its potential to persist and bioaccumulate. One of the most important determinants in predicting persistence and accumulation in biota and other environmental media is the partitioning behavior of the pollutant. Partitioning refers to where in the environment a chemical will tend to reside and in what relative quantities. When released to the air, chemicals may partition to air, water, soils, sediments, or biota, depending on a number of chemical and site-specific factors. Section 17.2 highlights measures of partitioning and other chemical and physical properties. Section 17.3 discusses how measures of persistence, bioaccumulation, and partitioning are used in exposure assessment.

17.1.1 Measures of Persistence

Estimating the persistence of chemicals in the environment is a challenging exercise. Persistence depends on basic processes such as how the chemicals are released (i.e., which environmental media they are released to initially, in this case, air); how they move in the environment (i.e., to which environmental media they tend to partition); and their tendency to degrade within those specific media (i.e., their persistence in air vs. in water). These basic processes, in turn, depend on a number of chemical-specific properties and site-specific conditions. However, despite the

complexity of the overall process, some general screening methods are available to get a sense of persistence of chemicals in certain media.

Within each environmental medium, several different degradation processes can influence the persistence of chemicals. However, regardless of the specific degradation process, what generally occurs is that organic chemicals (or organo-metallic compounds) are reduced in size and complexity, and, if complete degradation occurs, converted to carbon dioxide, methane, ammonia, water, sulfates, phosphates, nitrates, and other end products. Explanations of the specific degradation processes and their applications within different environmental media are summarized below and in Exhibit 17-1:

- **Aerobic biodegradation** is the breakdown of chemicals by microorganisms that utilize oxygen;
- **Hydrolysis** is the breakdown of chemicals by reaction with water;
- **Photolysis or photodegradation** is the process by which chemicals can be degraded by the energy in artificial light or sunlight;
- **Oxidation or reduction (or redox)** reactions involving the exchange of electrons between the pollutant and reactive compounds found in the environment;
- **Photooxidation** is a process by which oxidation and photolysis work jointly to break down chemicals and refers to a reaction with oxygen in the presence of light (usually sunlight); and
- **Anaerobic biodegradation** is the breakdown of chemicals by microorganisms without the use oxygen (for example, in sediments).

Persistence is usually described using a term called **half-life**, which is the time required for one-half of the original mass of the chemical to be degraded, transformed, or destroyed in a given medium. Half-life values may be measured directly or estimated (e.g., with computer models that predict half-life based on chemical structure). Alternatively, the literature may report a degradation or transformation **rate constant** in units such as 1/day or day⁻¹.

Assuming the reaction is first-order, the rate constant can be converted to the half-life and vice versa using the equation $t_{1/2} = 0.693/k$, where $t_{1/2}$ is the half-life (days) and k is the first-order rate constant (day⁻¹). Exhibit 17-2 provides a list of data sources for degradation half-life or rate constant values.

Exhibit 17-1. Degradation Processes in Environmental Media	
Environmental Medium	Applicable Degradation Process(es)
Air	Photolysis
	Photooxidation
Surface water	Aerobic biodegradation
	Hydrolysis
	Photolysis
	Photooxidation
Soils	Aerobic biodegradation
	Hydrolysis
	Photolysis (surface soil)
	Oxidation - reduction reactions
Sediments	Anaerobic biodegradation

Exhibit 17-2. Data Sources for Half-Life and Rate Constant Values

Data Source	Data Elements	Comments
Howard et al. Handbook	<ul style="list-style-type: none"> • High and low compartment half-life values for soil, air, surface water, and sediment/ground water based on measurements and modeling estimations; and • High and low measured and estimated process-specific half-life values, including hydrolysis, reduction, photolysis, photooxidation (in water and air), and biodegradation. 	Howard et al. ⁽¹⁾ compiled measured and estimated environmental degradation rates for organic chemicals, including polycyclic aromatic hydrocarbons (PAHs), pesticides, and solvents.
Mackay et al Handbooks	<ul style="list-style-type: none"> • Measured and estimated half-life and rate constant data for air, water, soil, and sediment. 	Mackay et al. ⁽²⁾ compiled measured and estimated environmental degradation rates for organic chemicals, including monoaromatic hydrocarbons, chlorobenzenes, polychlorinated biphenyls, polynuclear aromatic hydrocarbons, polychlorinated dioxins and dibenzofurans, volatile organic compounds (VOCs), pesticides, and oxygen, nitrogen, and sulfur organic compounds.
Verschuren	<ul style="list-style-type: none"> • Measured and estimated half-life values in surface water, ground water, sediment, soil, and biota. 	Verschuren ⁽³⁾ compiled measured and estimated degradation rates for organic chemicals.
Mercury Study Report to Congress	<ul style="list-style-type: none"> • Measured demethylation rate constants converted to half-life data for mercury (water, soil, sediment). 	The <i>Mercury Study Report to Congress</i> ⁽⁴⁾ was developed for a rulemaking and has undergone extensive Agency peer review.
HYDROWIN	<ul style="list-style-type: none"> • Estimated hydrolysis rate for water. 	HYDROWIN, the hydrolysis estimation program, is part of EPA's Estimation Program Interface (EPI) Suite. ⁽⁵⁾ HYDROWIN uses a chemical's structure to estimate the acid- and base-catalyzed rate constants for certain chemical classes (esters, carbamates, epoxides, halomethanes, and certain alkyl halides). Chemicals can be catalyzed (broken down) by acids (hydronium) or bases (hydroxide ions). The rate constants are used to calculate hydrolysis half-lives at selected pHs.

Half-life values for the same substance in different media, and for different substances in the same medium, can differ by several orders of magnitude. This is illustrated in Exhibit 17-3.

Exhibit 17-3. Example Illustrating Ranges of Half-life Values in Different Environmental Media				
HAP	Measured or Estimated Half-life Value (Hours)^(a)			
	Air	Water	Soil	Sediment
acrolein	19	672	672	1,776
benzene	276	252	252	9,984
chlorobenzene	401	2,616	50	1,800
formaldehyde	4	192	96	384
methyl bromide	8,980	420	420	1,680
2,3,7,8-TCDD	200	768	12,096	14,400
<i>Note: Values are for Illustrative Purposes Only</i>				
(a) Values represent the maximum measured or estimated values from the references cited in Exhibit 17-2.				

The fate and transport models used for characterizing multipathway exposure use metrics of persistence to account for loss of the chemical through degradation or transformation processes described above. Typically, for each modeled media compartment, the fate and transport models require an overall metric of persistence for that media compartment (e.g., a half-life value for air, a half-life value for soil, a half-life value for surface water). The media compartment half-life is the half-life associated with the most important or fastest degradation process or reaction. That is, the process-specific half-life of the fastest degradation process is usually selected as the overall media compartment half-life.

Metals may transform among different compounds or species (e.g., divalent mercury can undergo methylation to yield methyl mercury, and it can be reduced to form elemental mercury). Some metal species are more persistent and/or may be more toxic than others. Transformation half-life values in different media are more useful for evaluating the persistence of metal pollutants of concern. The speciation of metals is highly dependent on geochemical environment (and in some cases, the presence of certain microbes). One species may dominate in water of one pH, Eh, DOC concentration, etc., and an entirely different species may dominate in water of different geochemistry. [Also note that a further complicating factor is that analytical laboratories often report the total amount of a metal present in a sample, rather than the amount of the various individual metal species present (e.g., Cr^{6+} versus Cr^{3+}), which usually have different toxicities and different persistence values. An understanding of the concentrations of various metal species is therefore desirable; however, it is often not analytically achievable.]⁽⁶⁾ There are a number of concerns regarding the assessment of risks posed by metals in the environment. Information on this subject can be found at the following website:

<http://cfpub.epa.gov/ncea/raf/recordisplay.cfm?deid=51736>.

What is a Persistent Chemical?

Because environmental persistence is a complicated phenomenon, no single value is universally accepted as indicating a “persistent” chemical. EPA has used a half-life value of two months (1,440 hours) in the Toxics Release Inventory (TRI) PBT final rule and the Premanufacturing Notice evaluation process.⁽⁷⁾ Other authors have suggested a half-life value of one month (720 hours), using the following logic: Assuming that a chemical will degrade in approximately six half-lives (when less than two percent of the mass remains), a chemical with a half-life of one month would persist in the environment for six months. This six-month period would be long enough to encompass the sensitive developmental life stages of many organisms.⁽⁸⁾

Note that **the use of any single threshold value to define “persistent” chemicals may be misleading.** An important consideration is data quality (e.g., whether the half-life value is measured or predicted and the overall quality of the experimental study or computer algorithm used to develop the value). Assessors must consider other factors including the tendency of the chemical to partition into various media. For example, vinyl chloride has a half-life of six months in surface water and two years in sediment – values that might suggest this chemical is “persistent.” However, its half-life in air is 53.4 hours and in soil is 10 days. Thus, depending on its relative tendency to partition between air, soil, water, and sediment, a significant amount of the mass in air emissions might be degraded (in the air and/or soil) prior to the chemical reaching surface water and sediment.

Ultimately, it is often difficult to select a single and reliable half-life because the half-life of a chemical depends not only on its physical properties (see section 16.4), but also on the environmental conditions of the site to which the chemical is emitted. Temperature, sunlight intensity, the nature of the microbial community, and concentrations of reactive species such as oxygen radicals can all affect the reactivity of a compound.⁽³⁾

17.1.2 Metrics of Bioaccumulation

Several chemical-specific metrics can be used to evaluate the potential for a chemical to bioaccumulate in plants and animals and biomagnify in food webs.⁽⁹⁾ These values may be measured in laboratory tests or estimated with computer models based on chemical structure. These metrics include:

Note that BAFs and BCFs are not calculated for humans; rather, they are sometimes used to estimate air toxics concentrations in the food items eaten by people.

- **Bioaccumulation Factor (BAF).** The concentration of a substance in tissue of an organism divided by its concentration in an environmental medium in situations where the organism and its food are exposed (i.e., accounting for food chain exposure as well as direct chemical uptake). Such values are often used to characterize the transfer of pollutants through consumption of fish, beef, or dairy products.⁽¹⁰⁾
- **Bioconcentration Factor (BCF).** The concentration of a substance in the tissue of an organism divided by the concentration in an environmental medium (e.g., the concentration of a substance in an aquatic organism [$\mu\text{g/kg}$ body weight] divided by the concentration in the ambient water [$\mu\text{g/L}$ water], in situations where the organism is exposed through the water only). The most commonly given value is an estimate of the relative concentrations in water and whole fish (or, in some cases, fish fillets, since most people in the U.S. do not eat

whole fish), but BCFs for other organisms are also available. For plants, the Root Concentration Factor (RCF) indicates how readily pollutants are taken up from soil into underground tissues.

- **Octanol/water partition coefficient.** The ratio of a chemical's solubility in n-octanol to its solubility in water at equilibrium (in this test, n-octanol is used as a surrogate for lipophilic tissue). This metric, usually expressed as a logarithm ($\log K_{ow}$ or $\log P$), is often used as a surrogate for (and is an important basis for estimating) BAF or BCF.

As with persistence, bioaccumulation is a complicated phenomenon, and no single value is universally accepted as indicating that a chemical has a high tendency to bioaccumulate, although EPA's Office of Pollution Prevention and Toxics has used a threshold BCF value of 1,000 in evaluating new and existing chemicals.⁽¹¹⁾ Exhibit 17-4 provides a list of sources for bioaccumulation data.

Importance of Trophic Levels in Evaluating Bioaccumulation in Aquatic Food Chains

An organism's trophic position in the aquatic food web can have an important effect on the magnitude of bioaccumulation of certain chemicals. Certain pollutants have the potential to biomagnify, or increase in concentration at successive trophic levels through a series of predator-prey associations. Chapter 5 (Bioaccumulation) of EPA's *Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health* provides guidance about deriving trophic level-specific bioaccumulation factors.⁽¹⁷⁾

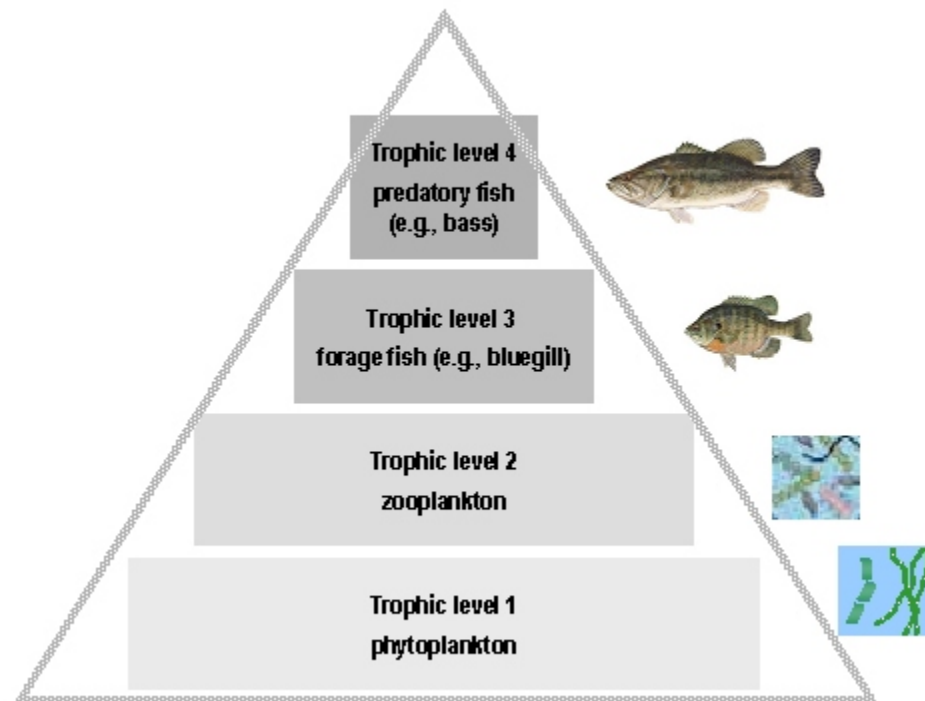


Exhibit 17-4. Sources of BCF and BAF Values		
Data Source	Data Element	Comments
HWIR Technical Support Document	Measured BAF Measured BCF Predicted BAF Predicted BCF	The Hazardous Waste Identification Rule (HWIR) Technical Support Document ⁽¹²⁾ data were developed for a rulemaking. Estimates are available for different classes of organisms (fish and invertebrates).
Mercury Study Report to Congress	Measured BAF for mercury	The <i>Mercury Study Report to Congress</i> ⁽⁴⁾ was developed for a rulemaking and has undergone extensive Agency peer review.
Ambient Water Quality Criteria documents	Measured BCF	Ambient Water Quality Criteria documents ⁽¹³⁾ are developed for rulemakings that establish concentration limits for chemicals in the surface waters of the United States. They have undergone extensive Agency peer review.
AQUIRE Database	Measured BCF	EPA's Office of Research and Development, Environmental Research Laboratory in Duluth, MN, maintains a database of citations and aquatic bioassay data including residue measures. ⁽¹⁴⁾
BCFWIN	Predicted BCF	BCFWIN, the Bioconcentration Factor Estimation Program, is part of EPA's EPI Suite. ⁽⁵⁾ This program estimates BCFs based on log K_{ow} data using the estimation methodology presented in a 1997 study prepared for EPA by Meylan et al. ⁽¹⁵⁾ The methodology was formulated using a training set of 694 compounds with measured BCF values for fish. In order of preference, the program uses (1) the log K_{ow} entered by the user, (2) the experimental log K_{ow} from the experimental log K_{ow} database for KOWWIN, and (3) the KOWWIN estimated log K_{ow} value.

BAF or BCF values are used in some fate and transport models to calculate how much of the chemical will partition into organisms, such as fish or shellfish, that are consumed by humans or ecological receptors of concern. The concentrations in these biota can then be used to calculate the intake of the chemical by humans or ecological receptors of interest. It is recommended that BAFs be derived separately for species of different trophic levels to account for different levels of accumulation for members of different trophic levels.⁽¹⁶⁾ EPA presents specific guidelines for deriving BAF values, including how to estimate BAFs using BCF values in its revised methodology for developing Ambient Water Quality Criteria.⁽¹⁷⁾ National-level BAFs developed by the Office of Water can be used in screening analyses. These can be refined based on site-specific characteristics in subsequent tiers of the assessment, if necessary.

As with half-life values, BCF values vary significantly among air toxics. Exhibit 17-5 presents a few representative BCF values for several HAPs. Note that these represent the highest values identified in the references cited in Exhibit 17-4 and are meant for illustrative purposes only.

Exhibit 17-5. Example BCF Values	
HAP	BCF Value ^(a)
acrolein	3
carbon tetrachloride	30
chloroform	6
pentachlorophenol	776
2,3,7,8-TCDD	5,754
<i>Note: values are for illustrative purposes only</i>	
(a) Values represent the maximum measured or estimated values from the references cited in Exhibit 17-4.	

Note that **the use of any single threshold value to define “bioaccumulative” chemicals may be misleading**. As with persistence, data quality is an important consideration (e.g., measured vs. predicted values; quality of the underlying study/algorithm used to develop the value). Moreover, the specific organisms and tissues in which bioaccumulation is measured or predicted are important determinants of the relevance of a given BCF or BAF value for the exposure assessment. Many substances that bioaccumulate tend to accumulate in lipid tissues (e.g., fat, organs), which may not be the tissues that most people eat (e.g., fish fillet). Therefore, a high BCF may not actually result in high exposures to humans.

17.2 Chemical and Physical Properties that Affect Persistence and Bioaccumulation

Exhibit 17-6 identifies both direct metrics of persistence (i.e., half-life values), as well as the physical and chemical properties that are most important in determining persistence and bioaccumulation.

In Exhibit 17-6, **solubility** and **vapor pressure** determine the propensity for pollutants to dissolve in water and volatilize into the air, respectively. The **Henry’s Law constant**, which is simply the ratio of the chemical’s water solubility to its vapor pressure, indicates whether a compound will partition into air or water at equilibrium. The speed with which the equilibrium occurs is affected by the diffusion constants in air and water.

The coefficients that are abbreviated with a capital “K” (e.g., the octanol-water partition coefficient, K_{ow}) in Exhibit 17-6 provide information on how strongly organic and inorganic compounds are likely to bind to soil or sediment particles, or to partition into lipid versus aqueous phase liquids. Strong binding indicates a high potential to persist and accumulate in soils and sediments; soil/sediment binding also tends to be correlated with the potential to bioaccumulate.

The 1998 Peer Review Draft of EPA’s *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities* (HHRAP) provides (Appendix A) tables of recommended rate constants and chemical/physical parameters for a large number of air toxics.⁽¹⁸⁾ Also, the user’s guide for EPA’s Risk Screening Environmental Indicators (RSEI) tool includes physicochemical properties for TRI chemicals and chemical categories.⁽¹⁹⁾ Note, however, the values in these sources may need to be updated.

Exhibit 17-6. Chemical and Physical Property Definitions

Property	Definition	Significance/Comments
Name	Unique identifier	Not always reliable (many synonyms)
CAS No.	Unique identifier	Much more reliable than the chemical name; some chemicals have no CAS number; some CAS numbers refer to mixtures
MW	Molecular weight	In absence of data, can be used to calculate D_a , D_w , etc.
V_p	Vapor pressure	Indicates volatility
S	Solubility	Indicates maximum concentration of a chemical that will dissolve in water
H	Henry's Law constant	Ratio of vapor phase concentration to the liquid phase concentration of a gas; high values indicate tendency to volatilize from water solution
D_a	Diffusion coefficient in air	Used to calculate rate of volatilization from air
D_w	Diffusion coefficient in water	Used to calculate rate of volatilization from water
K_{ow}	Octanol-water partition coefficient (log K_{ow} is frequently tabulated)	High value (> 1000 , $\log K_{ow} > 3$) indicates strong tendency to bioconcentrate
K_{oc}	Organic carbon partition coefficient (log K_{oc} often tabulated)	High value indicates strong tendency to bind to soil/sediment; K_{oc} , K_{ow} can be estimated from each other
Kd_{soil}	Soil dissociation constant	Indicates potential of inorganic ions/compounds to bind to soil; varies for different ionic species, pH, soil types
Kd_{sed}	Sediment dissociation constant	Indicates potential of inorganic ions/compounds to bind to sediment (similar to Kd_{soil})
$t_{1/2soil}$	Half-life in soil	Indicates persistence in soil; generally soil type, conditions, and degradation pathway(s) must be specified
$t_{1/2sed}$	Half-life in sediment	Indicates persistence in sediment; same considerations as for $t_{1/2soil}$
$t_{1/2sw}$	Half-life in surface water	Indicates persistence in surface water; for moderate to high-vapor pressure compounds
BAF	Bioaccumulation factor	Indicates accumulation of a compound into tissues of an organism from contact with contaminated water, contaminated sediments, and ingestion of contaminated food
BCF	Bioconcentration factor	Indicates accumulation of a compound into tissues of an organism from contact with a contaminated medium.
RCF	Root concentration factor	Ratio of root to soil concentration, measures propensity to take up pollutant from soil for defined plant species
B	Biotransfer factors	Describes propensity of pollutant to be transferred through food chain; defined for specific crops and consuming organisms (e.g., alfalfa => dairy cattle); generally correlates with BCF, K_{ow} ; used primarily for detailed pathway modeling

Fugacity as a Determinant in the Fate and Transport of a Pollutant

Once a contaminant is emitted from its source, the fate of the contaminant is determined by a number of factors (e.g., molecular weight, solubility, partition coefficients). In order to characterize the fate of the pollutant, modelers have developed the concept of fugacity⁽²⁰⁾ to define the tendency of the gas to escape to another phase in order to reach a steady-state equilibrium. This tendency to migrate then leads to partitioning of the pollutant across environmental media based on its chemical and physical characteristics. Fugacity models are distribution-based models incorporating all environmental compartments (media) and are used to quantify steady-state fluxes of pollutants across compartment interfaces. There exist three levels at which fugacity may be modeled. The Level I model depicts the distribution of a known quantity of a chemical in a closed environment at equilibrium, in which no degrading reaction occurs and no advective gain or loss is attained. A Level II model describes a situation in which a chemical is continuously discharged at a constant rate and achieves steady-state equilibrium, at which the input and output rates are equal. In Level II models, reaction and advection may occur. A Level III model is similar to a Level II model in that the modeled chemical is continuously discharged at a constant rate and achieves a steady state condition, in which the input rate equals the output rate. Yet, a Level III model differs in that fugacity for the given chemical is equal within a single compartment for all defined subcompartments, but is not equal between compartments. Therefore, individual inputs for each medium must be defined separately in order to determine appropriate pollutant partitioning among environmental compartments.

17.3 Evaluating Persistence and Bioaccumulation in Exposure Assessments

Characterizing the movements of air toxics that persist and which also may bioaccumulate through various environmental media such as air, soils, water, sediments, and biota can be a highly complex task, and generally available methods for evaluating these fate and transport pathways have only recently been developed. Specifically, EPA and other regulatory agencies have developed a number of models that estimate the concentrations of persistent and bioaccumulative compounds over time in the various environmental “compartments” subsequent to defined patterns of deposition. These models simulate both physical and chemical processes such as air deposition to soil, runoff, leaching (dissolution), soil/sediment adsorption, and chemical speciation (oxidation/reduction, precipitation reactions). Some models also evaluate the biodegradation of organic pollutants by bacteria and other organisms in soil, sediment, and surface water. These models require a large number of site-specific inputs and many measures of the physical and chemical properties of pollutants. It is beyond the scope of this chapter to discuss in detail all the processes that may be modeled in the assessment of indirect exposure pathways; however, Mackay and his colleagues provide a good overview of the multimedia fate and transport⁽²⁰⁾ and Conell and Emlay describe the principles governing the bioaccumulation of pollutants in the environment.⁽²¹⁾ Also, Chapter 18 provides a description of available multimedia models that are generally recommended for use in air toxics risk assessment. The documentation for these models provides detailed descriptions of the specific processes and methods used in each model.

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